Question 1

It is likely that mine detection dogs can only sniff the explosives that reside in the air (although there is some debate that they might also be able to inhale dust and detect sorbed explosives). It is therefore of interest to calculate the equilibrium air concentrations under various conditions. Calculate the partitioning of 2,4-dinitrotoluene (a by-product of TNT) in the following situations:

- For the training of the dogs it is necessary to use samples with different, well defined concentrations that can easily be prepared and reproduced in a standardized way. Aqueous solutions of 2,4-DNT might be a solution to this problem. Calculate the equilibrium air concentrations in a container that contained 3 mg DNT, 1 L water and 700 ml air. (Assume that there is no sorption to the walls of the vessel).

- While preparing a training sample the water got contaminated with some organic phase (e.g. oil, grease, solvent). Does this have a significant impact on the equilibrium air concentration? Use the numbers from above and assume that a contamination with 0.7 mg organic carbon occurs. Assume that you can use the $K_{oc\ w}$ value given below which has actually been determined for sorption in humic matter.

- In order to train animals for the REST procedure (see Chapter 2 for explanation) you spike various soils with 0.4 µg DNT: a) 3 g of air-dry soil (at 70 % rh) with an organic carbon fraction of 1 % (w/w), a water content of 9 % (w/w) and a mineral surface area of 40 m^2/g; b) 3 g of air-dry soil (at 90 % rh) with an organic carbon fraction of 3 % (w/w), a water content of 5 % (w/w) and a mineral surface area of 7 m^2/g; c) 6 g of wet soil (at 70 % rh) with an organic carbon fraction of 3 % (w/w), a water content of 30 % (w/w) and a mineral surface area of 40 m^2/g (assume that there is no adsorption to surfaces under wet conditions). These samples are placed in 20 ml containers. Calculate the equilibrium air concentrations in the closed containers assuming that the walls of the containers are inert.

- For the dogs to sniff at the samples the containers have to be opened of course. As a consequence, more air will get into contact with the sample. Assume that the soil will eventually equilibrate with 100 L of air before a dog gets to sniff on it. Does this have a substantial impact on the equilibrium air concentrations?

Use the following partition constants:

for DNT at 15°C:

- K_{wa} = 1.39 E5 [L_{air} /L_{water}]
- $K_{oc\ air}$ = 6.7 E7 [L_{air} /kg_{oc}]
- $K_{surface\ air}$ = 1.3 E-2 [m^3_{air} /$m^2_{surface}$] for mineral surfaces at 90% rH

and for TNT at 15°C:

- K_{wa} = 6.0 E6 [L_{air} /L_{water}]
- $K_{oc\ air}$ = 1.4 E5 [L_{air} /kg_{oc}]
- $K_{surface\ air}$ = 1.3 E-1 [m^3_{air} /$m^2_{surface}$] for mineral surfaces at 90% rH

Note, that the air/water partition constant is asked for in the spread sheet while the water/air partition constant has been given to you above.

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